Synopsis

This thesis investigates phonons and thermal transport in nanostructures In the wake of rapid development of small scale devices, thorough understanding of thermal transport phenomena is important to achieve tailored properties Despite numerous works, the theoretical understanding is far from complete Our aim is to understand phonon dynamics in nanostructures and propose a general model to predict size dependence of thermal transport properties There exist two cases of practical interest, in plane and cross plane thermal transport in nanoscale devices In this work we concentrate on the former

Using dynamical matrix formulation we investigate dispersion behavior of the phonon modes present in simple 2D nanostructures and compare with bulk phonon modes In our model bulk lattice is based on a square monoatomic unit cell, which is periodic in both x and y direction, with upto second nearest neighbor interaction The nanostructure has periodicity in x direction but is finite in y direction We define *thickness* or *size* of nanostructures as number of square unit cells present in y direction and also study the phonon modes as a function of thickness

We observe that in nanostructures there exist some additional phonon modes other than the modes already present in the bulk These modes are optical in nature and due to small group velocities contribute very lit-

tle in thermal energy transport in nanostructures The acoustic modes in the nanostructures are also significantly different from bulk acoustic modes Frequency of transverse acoustic(TA) mode is no longer a linear function of wavevector at small wavevectors, but rather exhibits a quadratic dependence As a consequence group velocity at small wavevectors is negligibly small and this mode no more contributes to thermal energy transport In the contrary frequency of longitudinal acoustic(LA) mode is a linear function of wavevector at small wavevectors As a consequence it has high group velocity and is the major contributor to the thermal energy transport in nanostructures LA branch in nanostructures shows a drastic deviation from bulk behavior at higher wavevectors Due to mode crossover phenomena, dispersion curve flattens suddenly within the first Brillouin zone and as a result group velocity decreases sharply at higher wavevectors

With increasing thickness, frequency of the phonon modes in the nanostructures increases and approaches to that of bulk Interestingly, this is found to be a function of second nearest neighbor interaction Frequencies of phonon modes in nanostructures with stronger second nearest neighbor interaction approaches bulk value with increasing thickness much slowly compared to modes in nanostructures with weaker second nearest neighbor interaction

Thermal transport property in solid is quantified by thermal conductivity(κ) and measurement of κ helps to get an insight into the physics of phonon dynamics We calculate the thermal conductivity of 3D nanostructures using equilibrium molecular dynamics simulation and Green-Kubo formulation We make a comparison between bulk and nanostructure thermal conductivity and also study it as a function of nanostructure thickness In our model nanostructures are based on FCC unit cell, bounded by (100) and (111) sur-

faces The constituent atoms interact via Lennard-Jones(LJ) potential, with parameters chosen to be that of solid argon Nanostructure thickness is defined by number of unit cells in z direction The solid is periodic in x and y direction We calculate κ in (100) and (111) plane for the two different class of nanostructures mentioned above

We observe that thermal conductivity in nanostructures is less compared to bulk thermal conductivity Further, thermal conductivity increases with increasing nanostructure thickness This is a consequence of change in phonon group velocity and relaxation time in nanostructures Phonon group velocity in nanostructures is different from that of bulk due to change in phonon dispersion relation On the other hand, surface to volume ratio plays an important role in determining the phonon relaxation time in nanostructures

Nanostructures, in particular thin films, generally contain some residual strain after deposition This can significantly affect thermal transport properties Hence we study the effect of strain on thermal conductivity in detail Again we use equilibrium molecular dynamics simulation and Green-Kubo formulation for the purpose of thermal conductivity measurement We take an unstrained FCC solid as our reference system, which is then subjected to homogeneous triaxial strain(both compressive and tensile) We use the same LJ argon potential for this study We observe that thermal conductivity decreases with increasing tensile strain Change of speed of sound(due to change in elastic constants as a function of strain) and phonon relaxation time play important in determining thermal conductivity With increasing tensile strain the system becomes more anharmonic, which leads to enhanced phonon-phonon scattering, leading to decrease in thermal conductivity

In summary - finite size can drastically affect phonon modes and relaxation times in a *systematic way*